Parallelization study of a VOF/Navier-Stokes model for 3D unstructured staggered meshes

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Abstract: The numerical simulation of interfacial and free surface flows is a vast and interesting topic in the areas of engineering and fundamental physics, such as the study of liquid-gas interfaces, formation of droplets, bubbles and sprays, combustion problems with liquid and gas reagents, study of wave motion and others.

One of the most powerful and robust methods for interface tracking on fixed grids is the Volume-of-Fluid (VOF). This method tracks the interface between different fluids by evolving the volume fraction scalar field, ratio of fluid to total volume, in time. First, the interface geometry is reconstructed from local volume fraction data. Then, the interface reconstruction and the solution of the Navier-Stokes equations are used to compute the volume fraction advection equation.

The objective of this work is to implement a fast, accurate and efficiently parallelizated VOF/Navier-Stokes model well suited to 3D unstructured staggered meshes. The interface will be reconstructed by a PLIC method and the advection step will be computed by the means of an unsplit-advection volume tracking algorithm. On the other hand, the Navier-Stokes equations will be solved using an unstructured staggered formulation.

The parallelization of the VOF/Navier-Stokes model will be studied by solving the Richtmyer-Meshkov instability (RMI). The Richtmyer-Meshkov instability occurs at a nearly planar interface separating two fluids that are impulsively accelerated in the direction normal to the interface. This impulsive acceleration can be the result of an impulsive body force or a passing shock wave.

Keywords: Multiphase flow, Volume-of-Fluid method, Unstructured Staggered Mesh, Parallelization.

1 Introduction

The contact of immiscible fluids or phases in motion, produces a thin region that separates them called interface. This kind of flows are called free surface or interfacial flows and are found in fields as varied as engineering, fundamental physics, geophysics and others. Typical examples of this phenomena are bubbles, drops, sprays, jets, waves, clouds, etc.

There are different methods for interface tracking, developed over the decades for specific problems, but the Volume-of-Fluid (VOF) [1] is one of the most widely used and successful in computational fluid dynamics for the simulation of interfacial and free surface flows. The VOF method mantains a sharp interface, preserves mass in a natural way and presents no problem for reconnection or breakup of the interface. This work, uses the VOF method presented by Jofre et al. [2].

When modelling multiphase systems, large discontinuities in the body force field typically appear at the interface. If the VOF method and a collocated mesh scheme [3] are used, such strongly variable body forces can produce unphysical spikes in the velocity field due to a checkerboard pressure field, then, a staggered mesh scheme [4] must be used. In this work, an unstructured staggered mesh scheme is developed from the formulation of Perot [5] and implemented on an accurate and parallelizable algorithm for 3D unstructured meshes.

2 Governing equations

In the VOF method, if the flow is assumed to be incompressible, the volume fraction C_k is evolved by the advection equation

$$\frac{\partial C_k}{\partial t} + \nabla \cdot (C_k \mathbf{u}) = 0 \tag{1}$$

and mass and momentum conservation are defined as

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot (\mu (\nabla \mathbf{u} + \nabla^T \mathbf{u})) + \mathbf{F}, \tag{3}$$

where $\mathbf{u}$ is the velocity field, p the pressure, $\mathbf{F}$ any body force, ρ and μ are the fluid density and viscosity, respectively, evaluated as

$$\rho = \sum_k \rho_k C_k \quad \text{and} \quad \mu = \sum_k \mu_k C_k \tag{4}$$

and subscript k refers to fluid k.

The solution of the momentum equation, Eq. (3), provides the velocity field used in the volume fraction advection equation, Eq. (1), to calculate the new volume fraction scalar field. Then, the new volume fraction field is introduced in the momentum equation to obtain the new velocity field.

3 Paralellization tests: Richtmyer-Meshkov instability

The Richtmyer-Meshkov instability (RMI) [6, 7] occurs at a nearly planar interface separating two fluids that are impulsively accelerated in the direction normal to the interface, regardless of whether the acceleration is directed from the heavy fluid to the light fluid, or vice versa. This impulsive acceleration can be the result of an impulsive body force or a passing shock wave.

A three-dimensional RMI is simulated in an effort to reproduce the flow features reported by Chapman and Jacobs [8]. The dimensions of the square tank are 72.6 *mm* x 72.6 *mm* in width and 250 *mm* in height. The lighter upper fluid and the heavier bottom fluid have an Atwood number equal to 0.15, the wavelength λ is 48.4 *mm*, the initial amplitude is calculated as $a_0 = 0.38/k$ and the initial disturbance is approximated by $\eta = a_0[\sin(kx) + \sin(ky)]$. The evolution of the interface separating the two fluids of the RMI simulation, calculated by the numerical model implemented in this work on a 250000 cell mesh, is shown in Fig. 1.

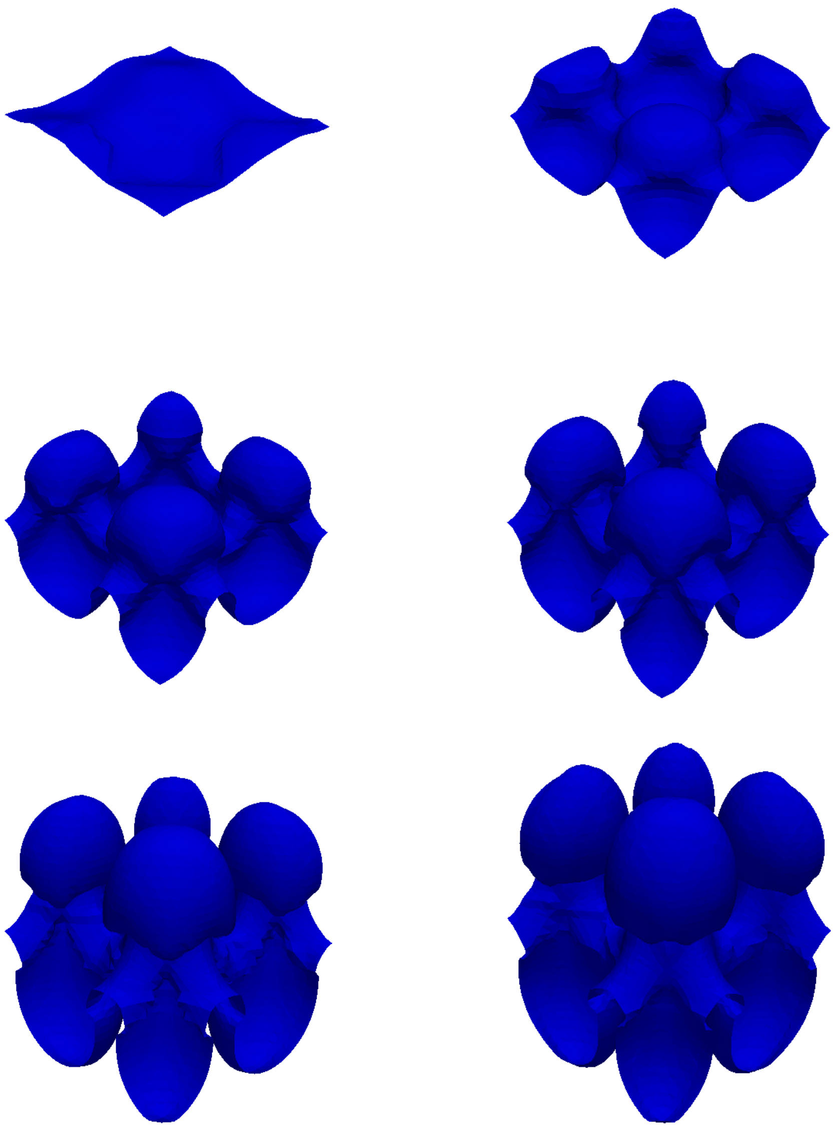

Figure 1: A sequence of images showing the evolution of the interface separating the two fluids of the RMI simulation.

In order to test the parallelization performance, two different partition configurations are chosen (see Fig. 2):

- Giving the same weight to all the cells, then, the partition algorithm partitionates the mesh creating cubes. In this way, the partitions are not adapted to the interface.
- Setting different weights to the cells to adapt the partition to the interface. With this strategy, partitions perpendicular to the interface are generated.

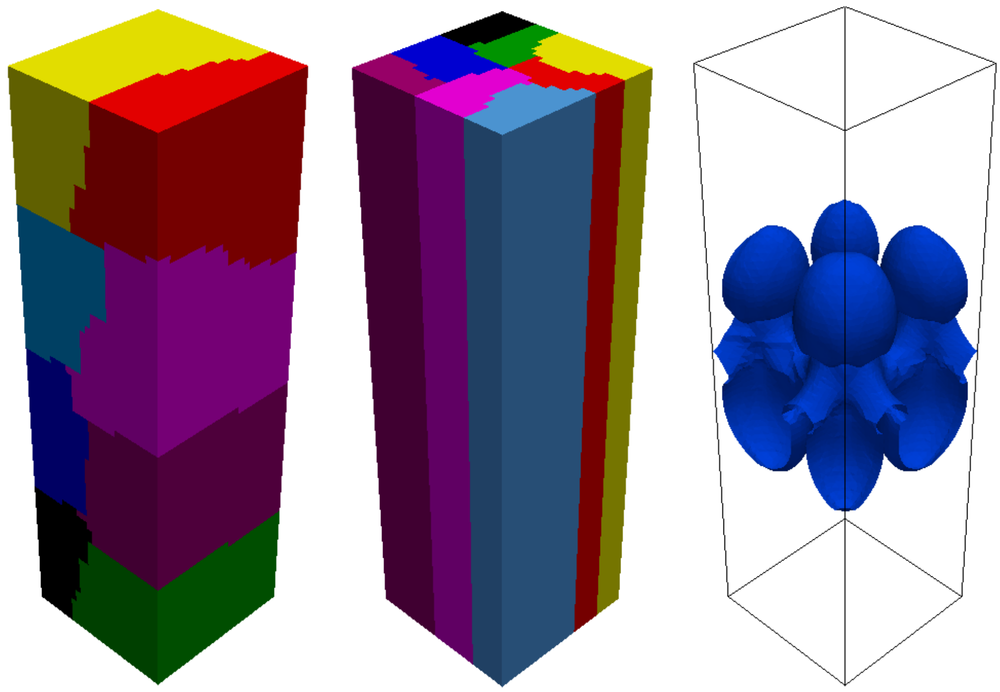

Figure 2: Sketches of the not adapted (left) and adapted (center) mesh partition configurations and the position of the interface related to the partitions (right).

The VOF phase time and the overall time (VOF + Navier-Stokes) per time step for the different partition configurations are plotted in Fig. 3.

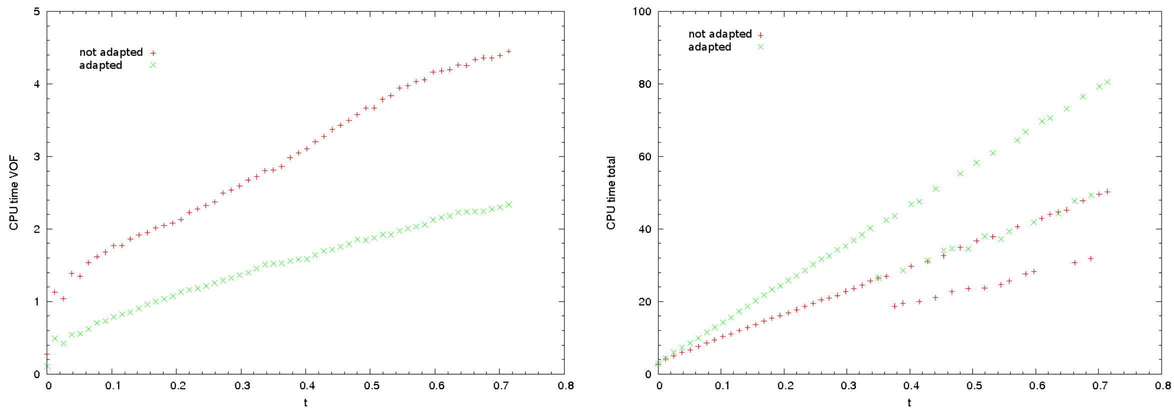

Figure 3: VOF and overall time for CPU over simulation time.

The results show that the partition adapted to the interface performs better in the VOF phase, but if we also take into account the Navier-Stokes calculation the total time is higher. This is because, the new partitions produce subdomains with larger boundaries. Thus, more information must be exchanged between processors on the Navier-Stokes calculations. These results suggest the need to work with different parallelization strategies for each of the parts of the algorithm: while we use a domain decomposition based strategy for the Navier-Stokes phase, we may use a mesh-partition independent strategy to solve the VOF phase. We are working in this new approach and it will be presented in the conference and final paper.

4 Conclusion and future lines

Traditional CFD parallelizations do not work well for VOF/Navier-Stokes models as it has been shown by solving the Richtmyer-Meshkov instability. The Navier-Stokes algorithm loads the CPUs in a balanced manner, but the VOF method loads the CPUs in a clearly desbalanced configuration (depends on where the interface is located). Therefore, the objective of this work is to develop and implement a new parallelization methodology for the VOF phase. This new method will balance the VOF load by distributing the work of the interface cells through all the CPUs independently of the mesh partition.

References

[1] C. W. Hirt and B. D. Nichols. Volume of fluid (VOF) Method for the Dynamics of Free Boundaries. *Journal of Computational Physics*, 39(5):201–225, 1981.

[2] L. Jofre, O. Lehmkuhl, J. Castro, and A. Oliva. A PLIC-VOF Implementation on Parallel 3D Unstructured Meshes. In *Proceedings of the Fifth European Conference on Computational Fluid Dynamics ECCOMAS CFD 2010*, 2010.

[3] C. M. Rhie and W. L. Chow. Numerical Study of th Turbulent Flow Past an Airfol with Trailing Edge Separation. *AIAA Journal*, 21:1525–1532, 1983.

[4] S. V. Patankar. *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing Corporation, 1980.

[5] B. Perot. Conservation Properties of Unstructured Staggered Mesh Schemes. *Journal of Computational Physics*, 159:58–89, 1999.

[6] R. D. Richtmyer. Taylor Instability in Shock Acceleration of Compressible Fluids. *Communications on Pure and Applied Mathematics*, 13(2):297–319, 1960.

[7] E. E. Meshkov. Instability of the Interface of Two Gases Accelerated by a Shock Wave. *Izv. Ross. Akad. Nauk, Mekh. Zhidk. Gaza*, 4(5):101–104, 1969.

[8] P. R. Chapman and J. W. Jacobs. Experiments on the Three-Dimensional Incompressible Richtmyer-Meshkov Instability. *Physics of Fluids*, 18(7), 2006.